

Ligand-breeding procedure

FIG. 1

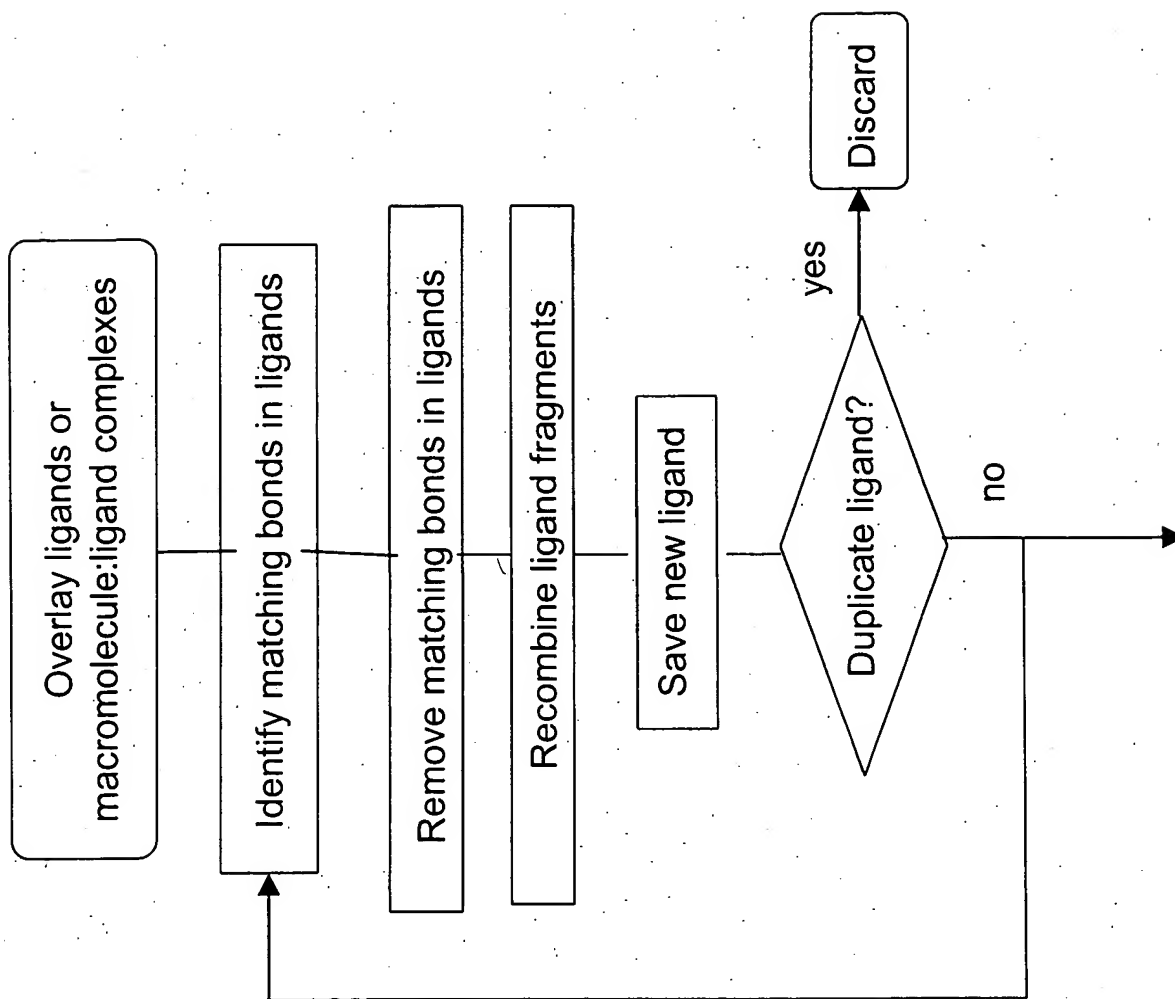
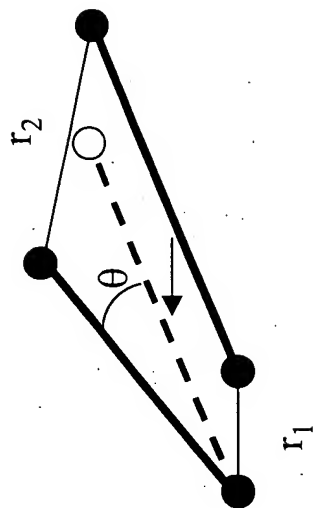


FIG. 2



Dark circles represent atoms, thick lines represent bonds. Thin lines show r_1 and r_2 , the distances between the atoms at each end of the bond. The dashed line shows the right-hand bond translated left so that the angle between the two bonds, θ , can be calculated.

FIG.3

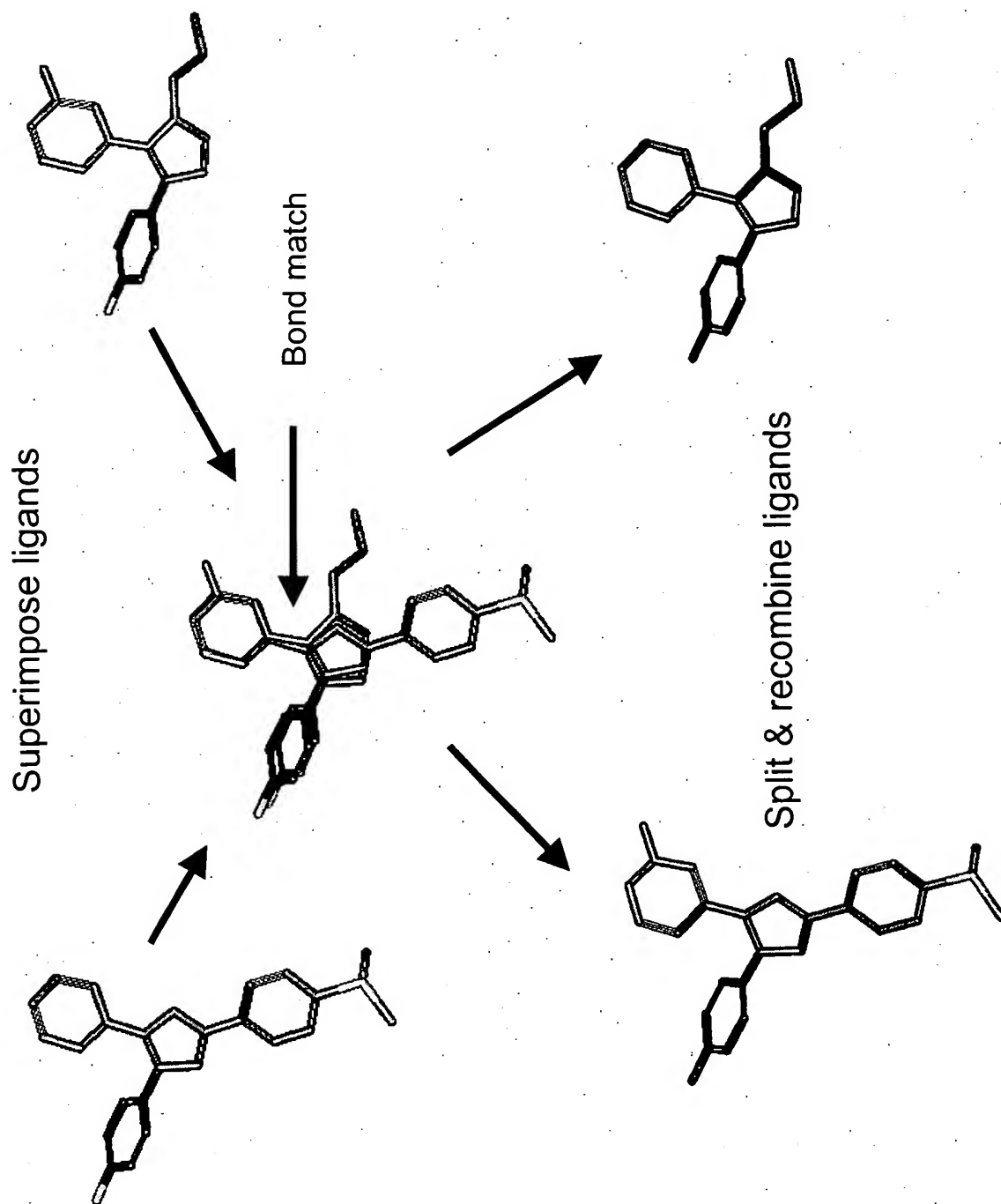
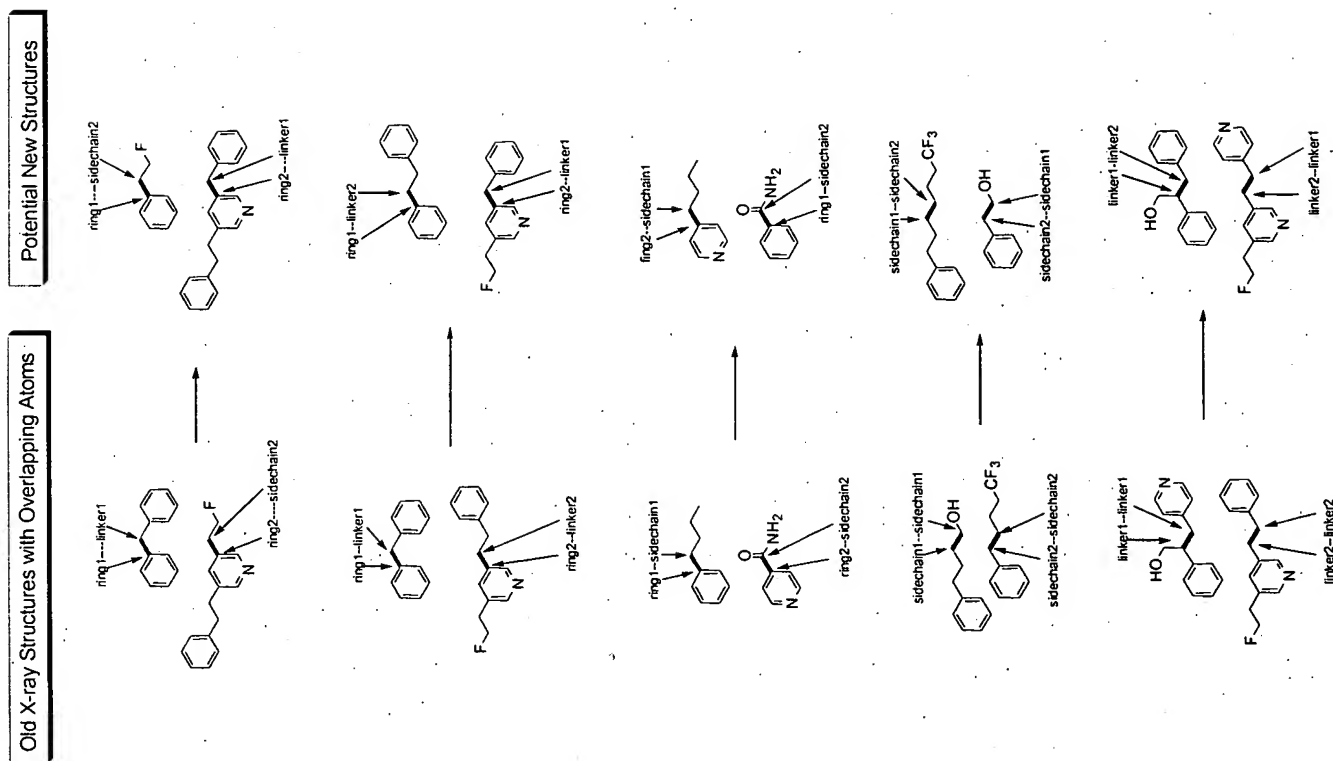


FIG. 4



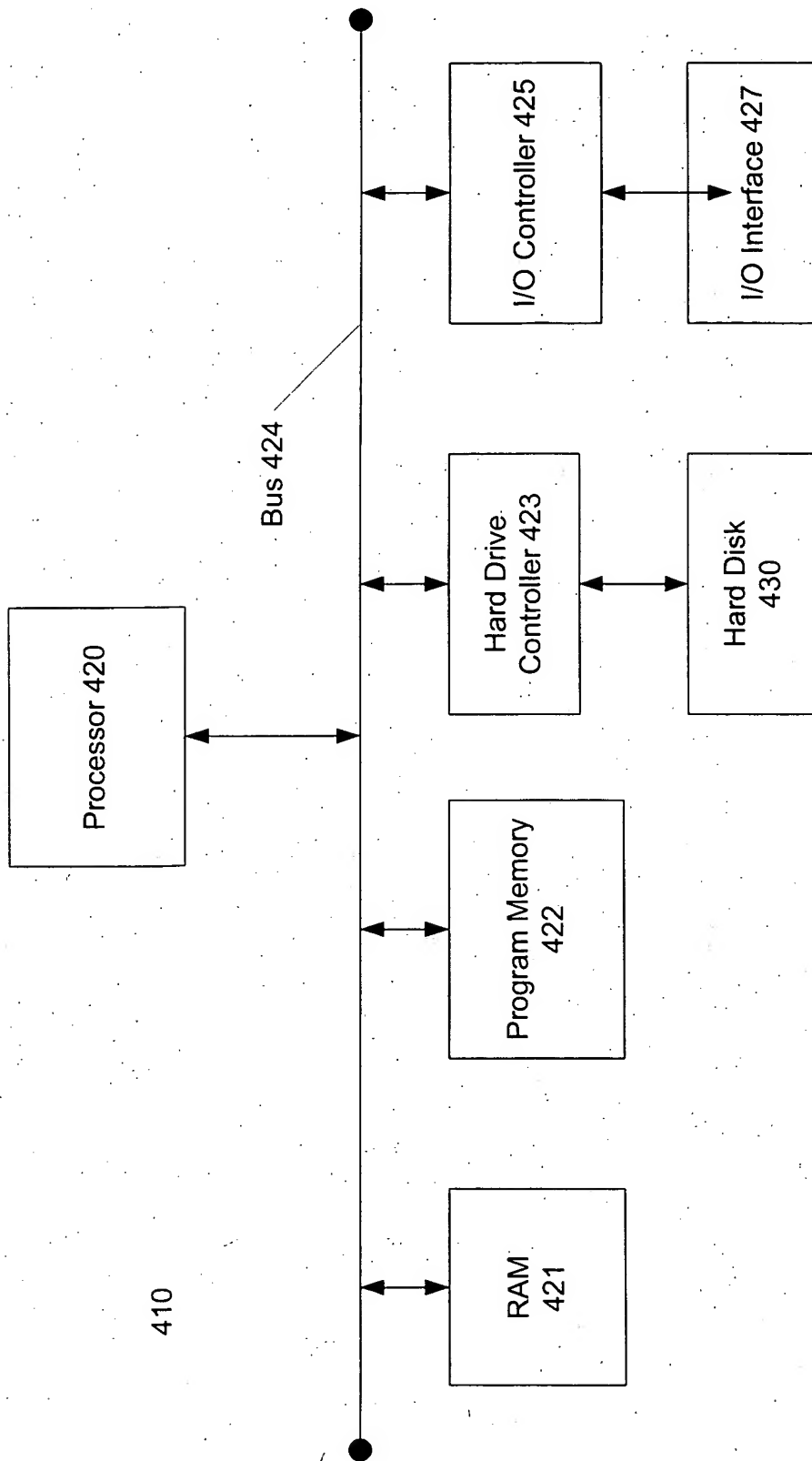


FIG. 5

FIG. 6

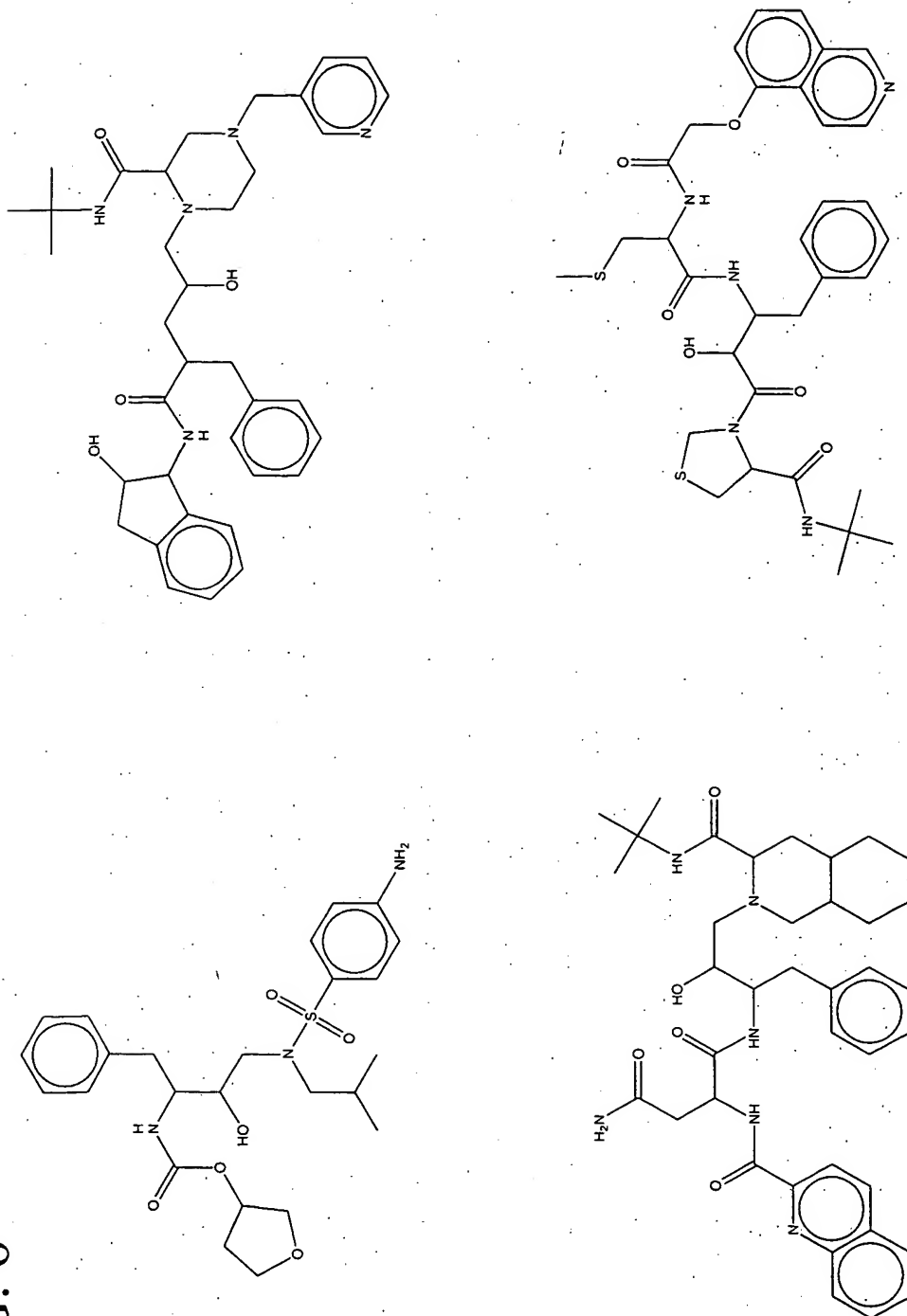


FIG. 7

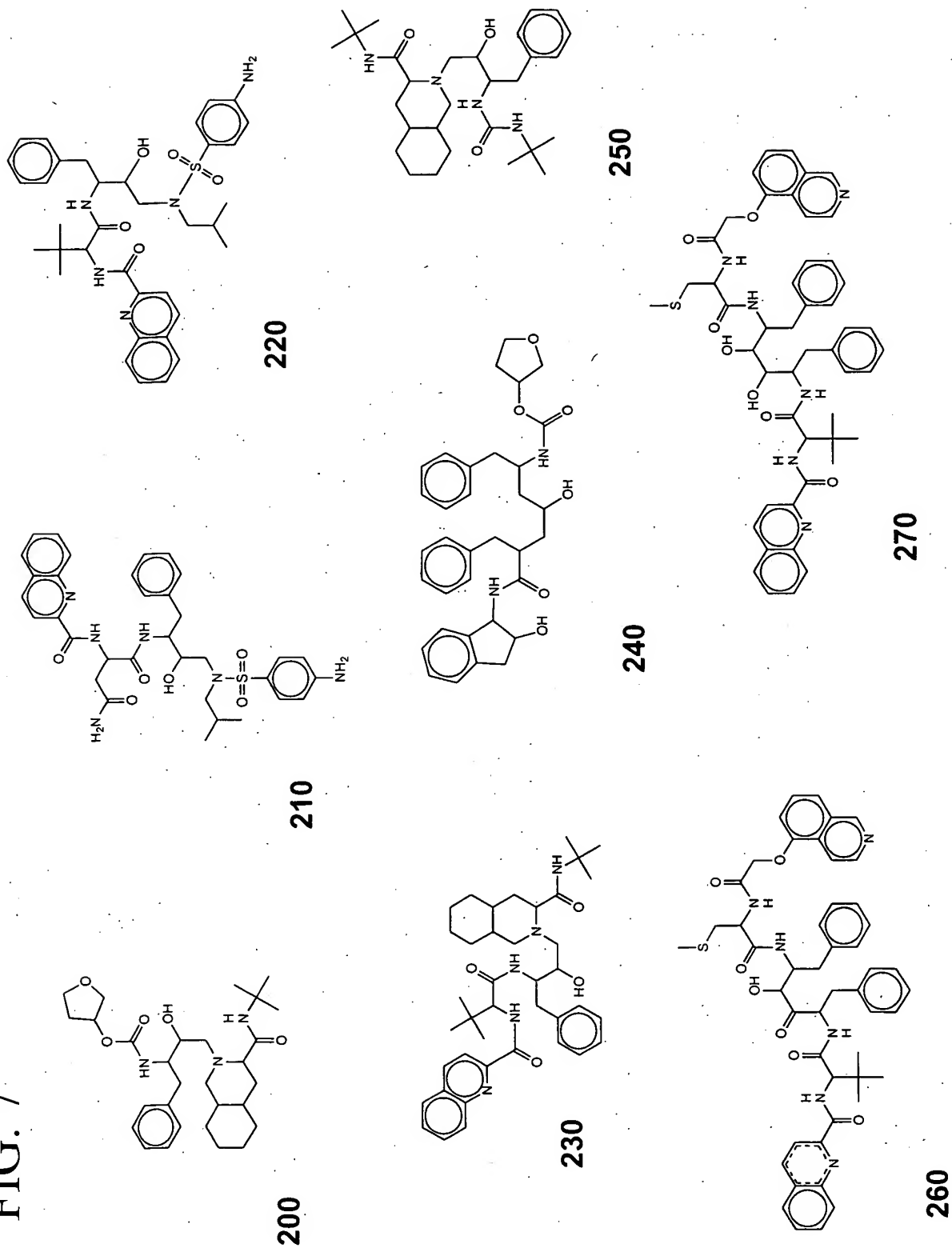
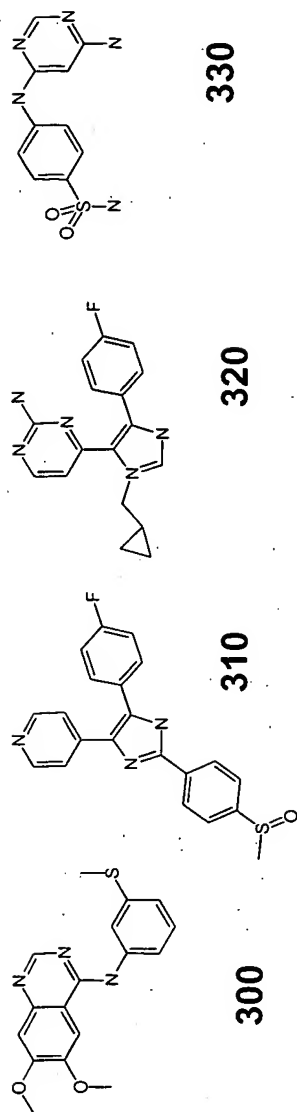


FIG. 8

Starting ligands



Output ligands

